

1-Chloro-2,6-diisopropyl-4-methylbenzene

Inchi:	InChI=1S/C13H19Cl/c1-8(2)11-6-10(5)7-12(9(3)4)13(11)14/h6-9H,1-5H3
InchiKey:	WURDTYCULJKTHQ-UHFFFAOYSA-N
Formula:	C13H19Cl
SMILES:	<chem>Cc1cc(C(C)C)c(Cl)c(C(C)C)c1</chem>
Mol. weight [g/mol]:	210.74
CAS:	98184-19-1

Physical Properties

Property code	Value	Unit	Source
gf	125.29	kJ/mol	Joback Method
hf	-135.83	kJ/mol	Joback Method
hfl	-194.00 ± 5.10	kJ/mol	NIST Webbook
hfus	19.45	kJ/mol	Joback Method
hvap	52.40	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.895		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
tb	575.01	K	Joback Method
tc	787.98	K	Joback Method
tf	300.17	K	Joback Method
vc	0.693	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.47	J/molxK	575.01	Joback Method
cpg	442.06	J/molxK	610.51	Joback Method
cpg	457.77	J/molxK	646.00	Joback Method
cpg	472.61	J/molxK	681.50	Joback Method
cpg	486.62	J/molxK	716.99	Joback Method
cpg	499.82	J/molxK	752.49	Joback Method
cpg	512.24	J/molxK	787.98	Joback Method
dvisc	0.0022241	Paxs	300.17	Joback Method

dvisc	0.0010689	Paxs	345.98	Joback Method
dvisc	0.0006098	Paxs	391.78	Joback Method
dvisc	0.0003912	Paxs	437.59	Joback Method
dvisc	0.0002730	Paxs	483.40	Joback Method
dvisc	0.0002028	Paxs	529.20	Joback Method
dvisc	0.0001579	Paxs	575.01	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98184191&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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